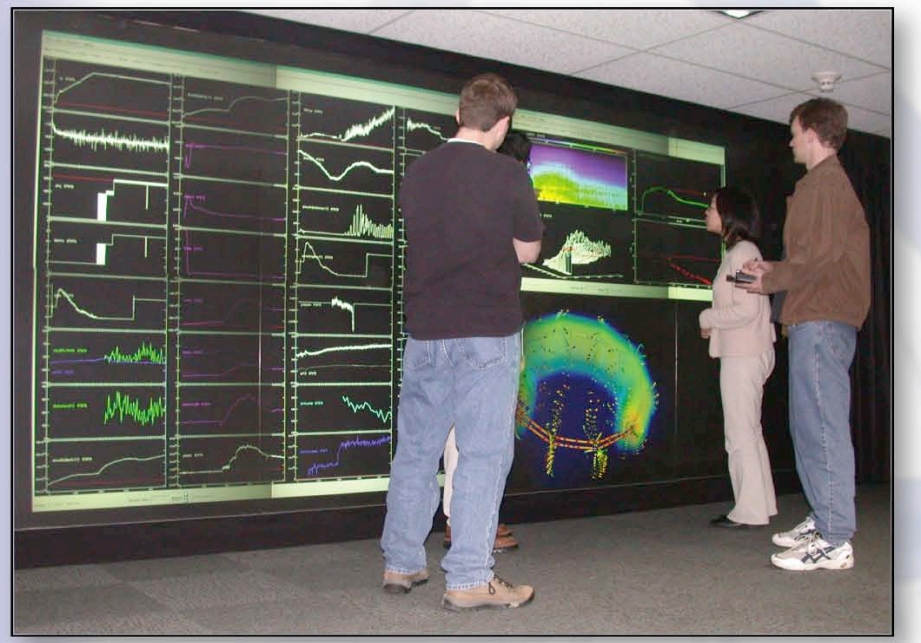
Grid Computing and Collaboration Technology in Support of Fusion Energy Sciences



by
David P. Schissel

Presented at
46th Annual Meeting of the
Division of Plasma Physics
Savannah, GA

November 15–19, 2004

GENERAL ATOMICS

ACKNOWLEDGMENT

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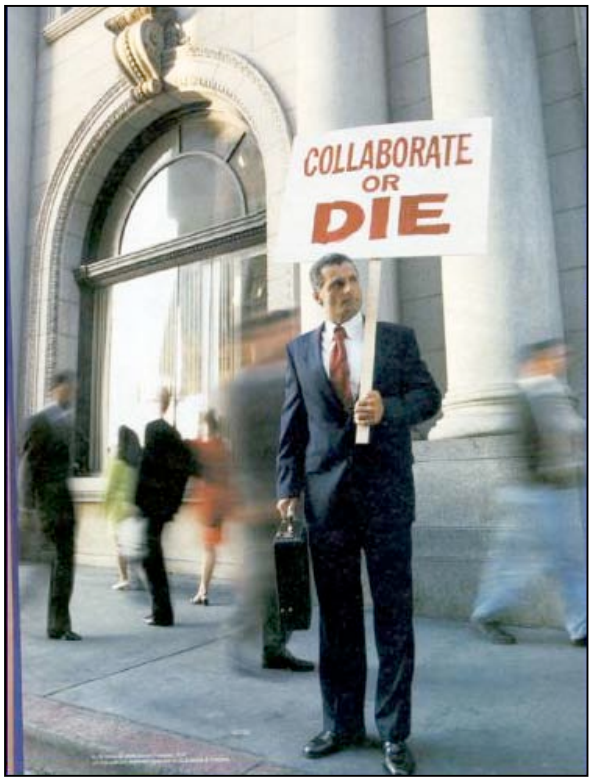
  - Office of Fusion Energy Sciences
  - Office of Advanced Scientific Computing Research

Office of Science
U.S. DEPARTMENT OF ENERGY

GENERAL ATOMICS

TUTORIAL'S KEY POINTS

- Scientific progress depends increasingly on large-scale distributed collaborative work
  - High energy physics at CERN or fusion with ITER
- Such distributed collaborative work raises challenging problems of broad importance
  - Cross-disciplinary community of technology producers and consumers required
- Large world-wide effort for solutions
  - Will effect your future working environment



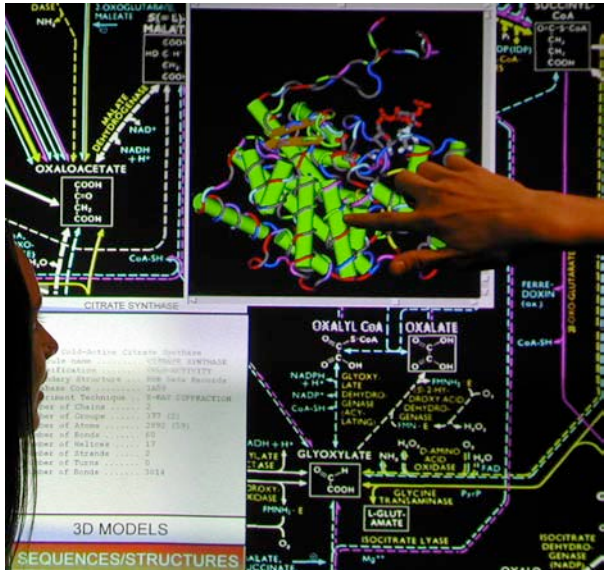
- Demonstrations of today's technology in the poster room
  - Learn more detail, get involved, and provide feedback

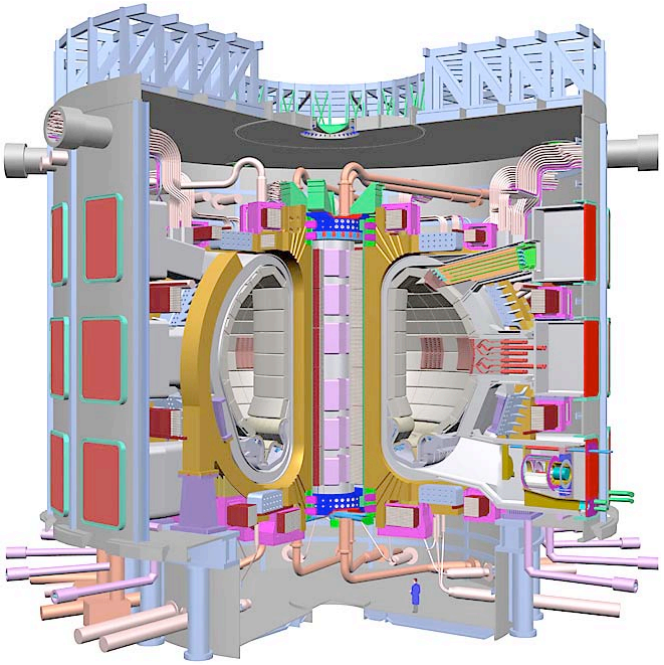
GENERAL ATOMICS

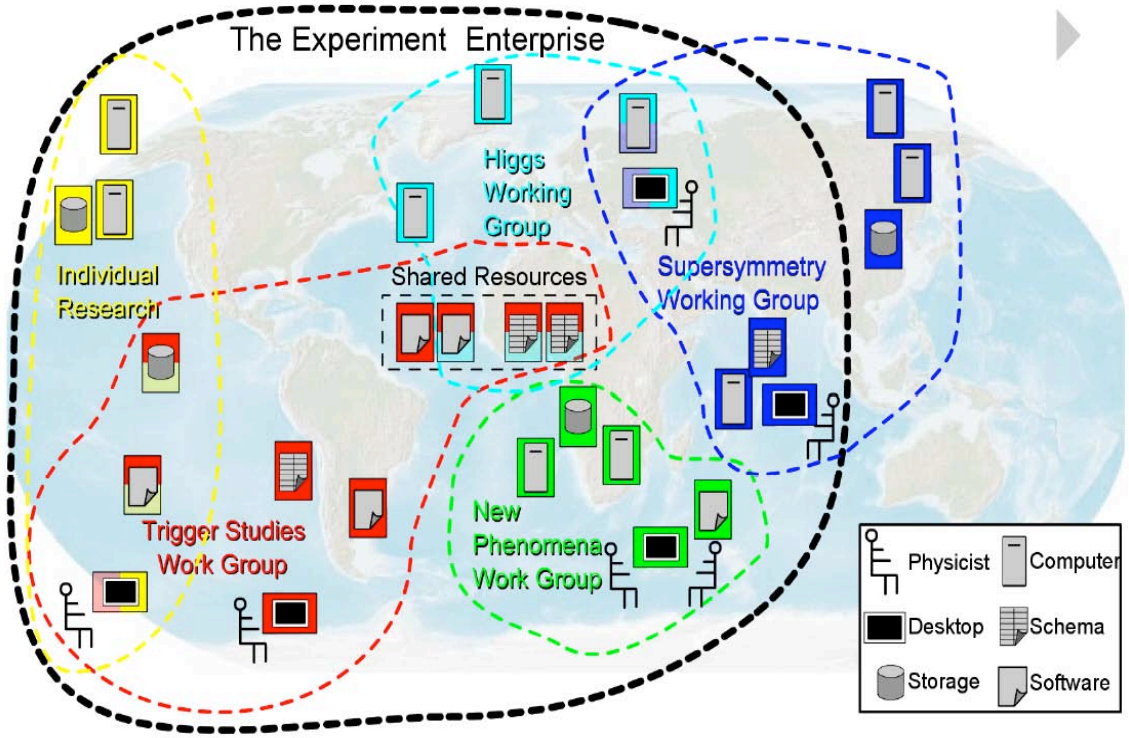
TUTORIAL'S OUTLINE

- Motivation for Collaborative Research
  - Science is more and more a team activity
- Grid Computing
  - Resource sharing and coordinated problem solving in a virtual organization
- Security
  - Allowing resource providers to control resources they give to the Grid
- Data Management
  - Where is that piece of data?
- Computation and Visualization
  - Compute and see the data for understanding
- Advanced Collaborative Environments (ACE)
  - Productive distributed group work
- Grid and ACE technologies applied to fusion research
  - The National Fusion Collaboratory Project

SCIENCE TODAY IS A TEAM SPORT

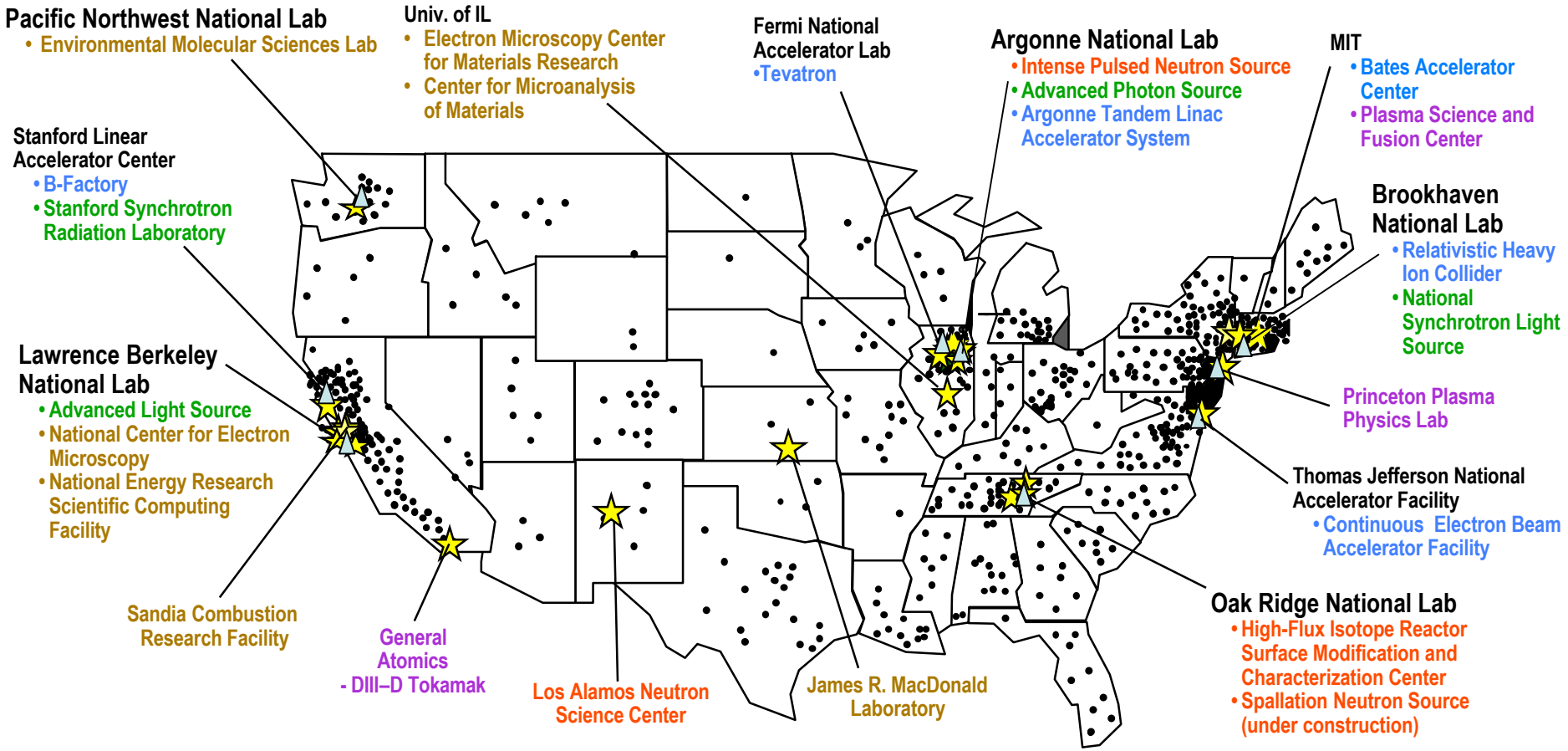






GENERAL ATOMICS

SCIENCE AS A TEAM SPORT PARTICULARY WITHIN DOE



SC Laboratories

SC User Facilities

Institutions that Use SC Facilities

- Physics Accelerators
- Synchrotron Light Sources
- Neutron Sources
- Special Purpose Facilities
- Large Fusion Experiments

GENERAL ATOMICS

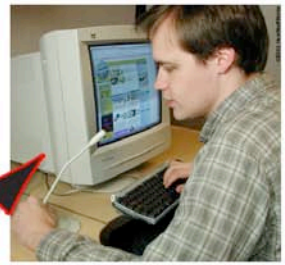
CHALLENGES FOR 21ST CENTURY DOE SCIENCE

- Scientific excellence in the context of
  - Unique facilities
  - Complex problems
  - Enormous data
  - Distributed teams
  - Multidisciplinary research
  - International in scope

GENERAL ATOMICS

MUST BE ABLE TO ASSEMBLE REQUIRED EXPERTISE AND RESOURCES WHEN NEEDED

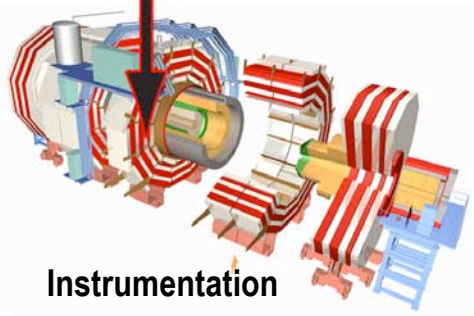
High-Performance Computation



Broadband Network Connectivity

Large Databases Digital Libraries

People and Training



Instrumentation

Transform resources into on-demand services accessible to any individual or team

GENERAL ATOMICS

PLACING DISTRIBUTED COMPUTING APPLICATIONS ON THE WIDE AREA NETWORK PRESENTS SIGNIFICANT CHALLENGES

- Crosses administrative boundaries
- Increased concerns and complexity for security including authentication and authorization
- Resources not owned by a single project or program
- Distributed control of resources by owners is essential
- Needs for end-to-end application performance & problem resolution
  - Resource monitoring, management & troubleshooting not straightforward
  - Higher latency challenges network throughput & interactivity
- People are not in one place for easy communication

GENERAL ATOMICS

GRID COMPUTING

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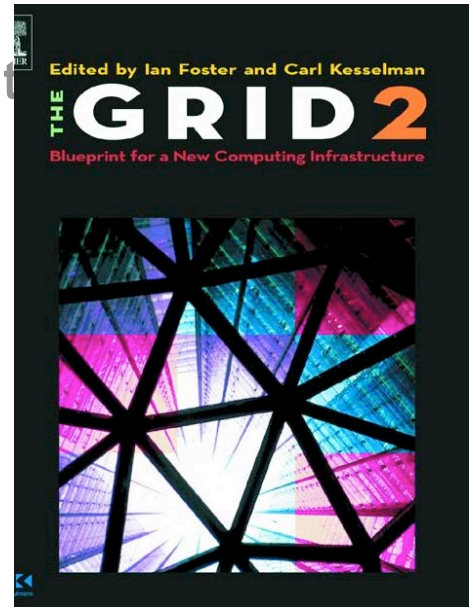
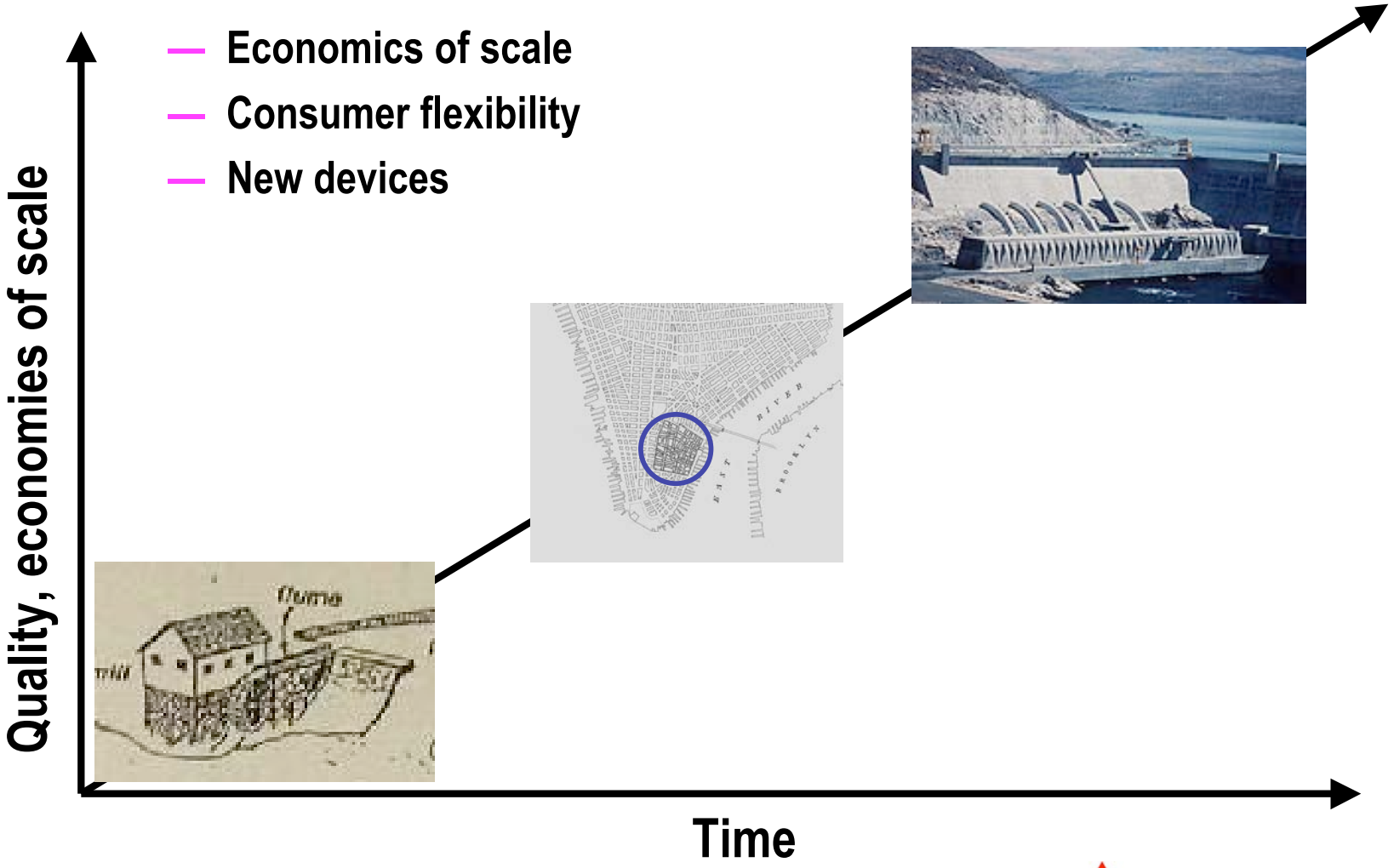


GENERAL ATOMICS

THE GRID IDEA: ON DEMAND ACCESS AS ENABLER

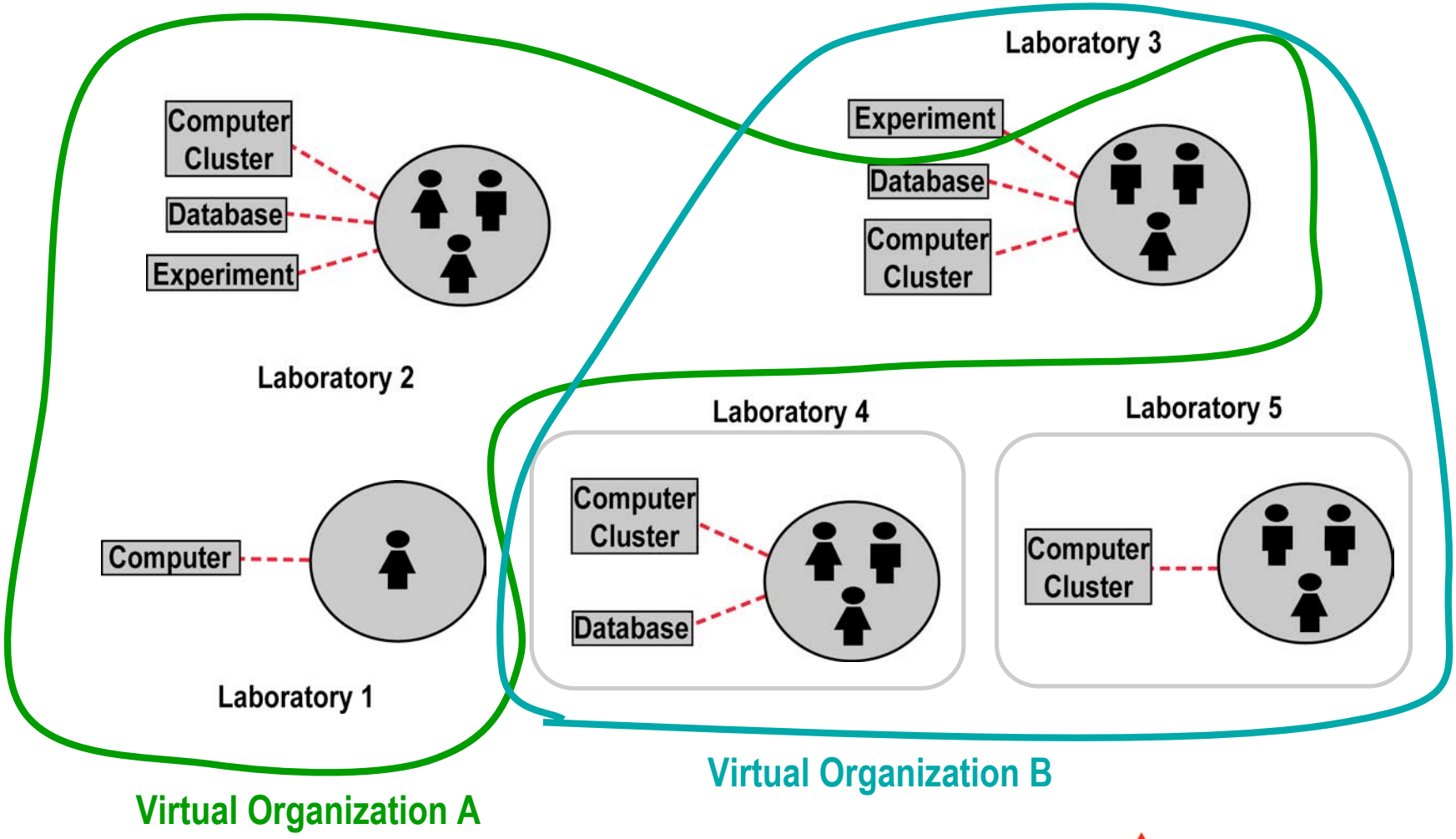
- Decouple production & consumption, enabling
  - On-demand access
  - Economics of scale
  - Consumer flexibility
  - New devices



GENERAL ATOMICS

THE UNIFYING CONCEPT: THE GRID

"Resource sharing and coordinated problem solving in dynamic, multi-institutional virtual organizations."



GENERAL ATOMICS

EXAMPLES OF BASIC GRID SERVICES

- Using remote computing power (resource management)
  - Tools for remote job and resource management
  - Schedulers, meta-schedulers, etc.
- Security services
  - Authentication based on Grid-wide credential
  - Single sign-on, delegation
  - Authorization
- Discovery and monitoring services
  - Grid-wide information on the state of resources
- Data Grid technologies
  - Secure and efficient data transfer
  - Managing replicas in the Grid
  - Virtual data

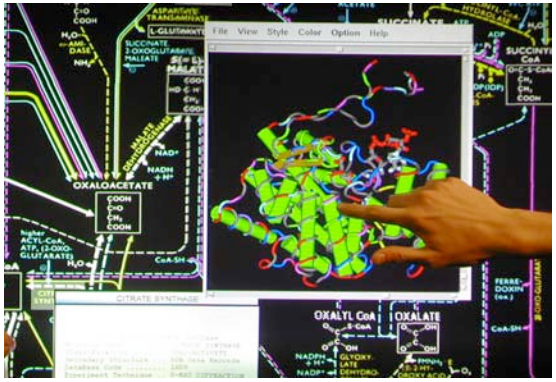
Global Grid Forum

– Setting Standards
– 450 people, 35 countries

GENERAL ATOMICS

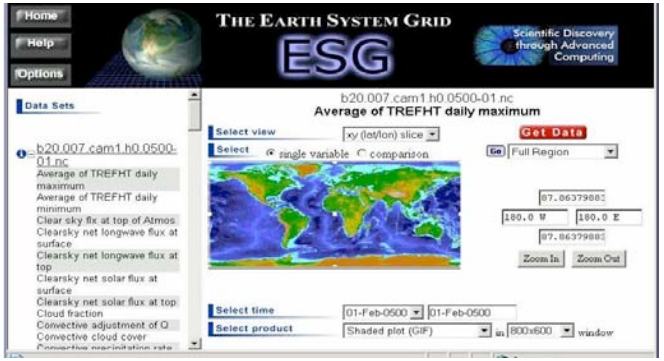
EXAMPLE GRID CAPABILITIES

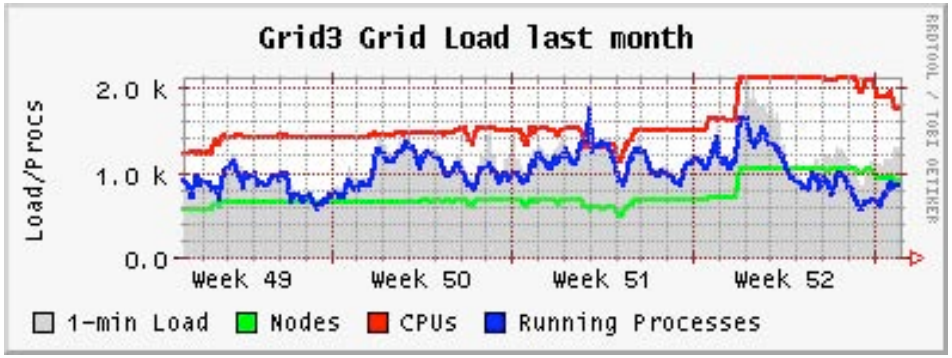
Engage via telepresence in an experiment at a remote facility



Discover and access a genome analysis service (analysis code running on a high-end computer)

Integrate data from multiple sources in support of global change research

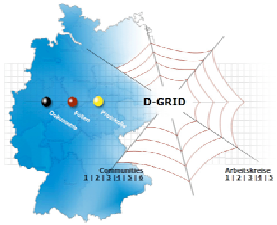


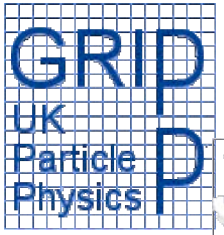


Harness computers across sites to process data from a physics experiment

GENERAL ATOMICS

GRID: ENABLER OF SCIENCE





EXAMPLE GRID INFRASTRUCTURE: NSF FUNDED NETWORK FOR EARTHQUAKE ENGINEERING SIMULATION (NEES)

Laboratory Equipment

Remote Users

Instrumented Structures and Sites

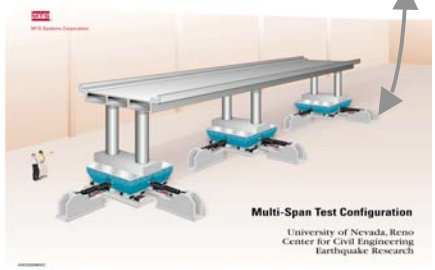
Simulation Tools Repository

High-Performance Network(s)

Field Equipment

Curated Data Repository

Global Connections



Laboratory Equipment

Large-scale Computation

Remote Users: (K-12 Faculty and Students)

NEESgrid

GENERAL ATOMICS

GRID: STARTING TO BECOME AN ENABLER OF INDUSTRY

Leading adopters (October 2003)
- **Financial services: 31%**
- **Life sciences: 26%**
- **Manufacturing: 18%**

Grids 2004: From Rocket Science to Business Service, The 451 Group

"All computers (and computer users) will join the grid."
- Seven Shifts that will transform the Future, IBM 2001 Annual Report

GENERAL ATOMICS

SECURITY IN THE CONTEXT OF GRID COMPUTING

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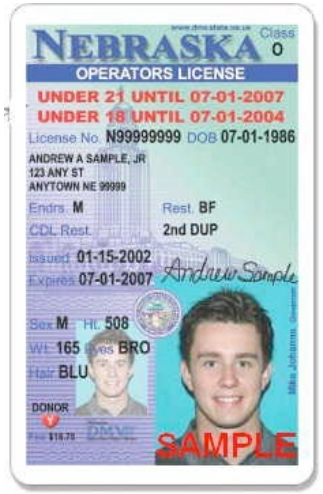
GENERAL ATOMICS

SECURITY IN A VIRTUAL ORGANIZATION IS A CHALLENGING PROBLEM

- **Authentication**
  - The receiver of a digital request must be confident of both the identity of the sender and the integrity of the message
- **Authorization**
  - Upon validating the identity of the requestor, should the request be allowed?

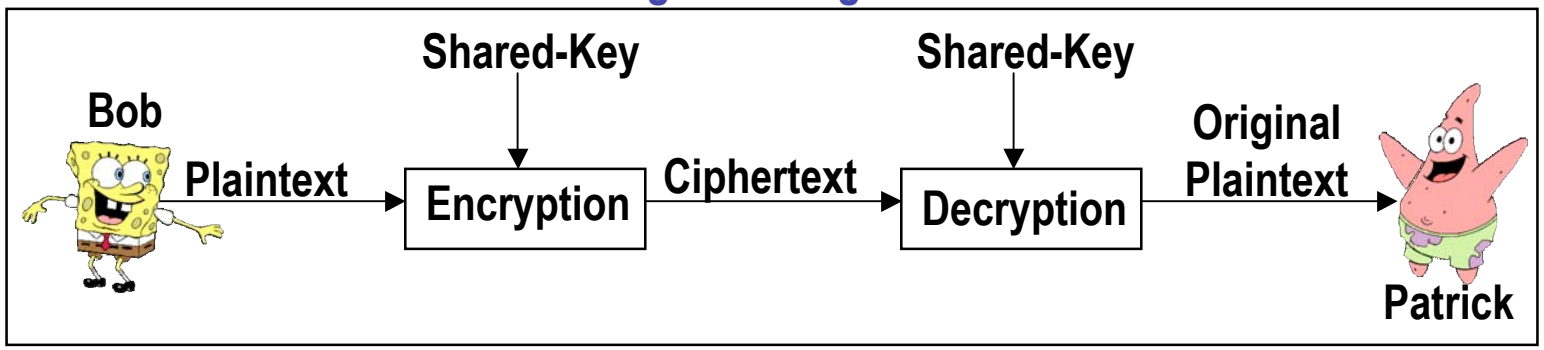


	Answers the question	Analogy
Authentication	Who are you?	Drivers License
Authorization	Do you have permission?	Plane Boarding Pass

GENERAL ATOMICS

HOW DO YOU VERIFY IDENTITY WHEN TWO PEOPLE DO NOT PHYSICALLY INTERACT?

Bob sending a message to Patrick

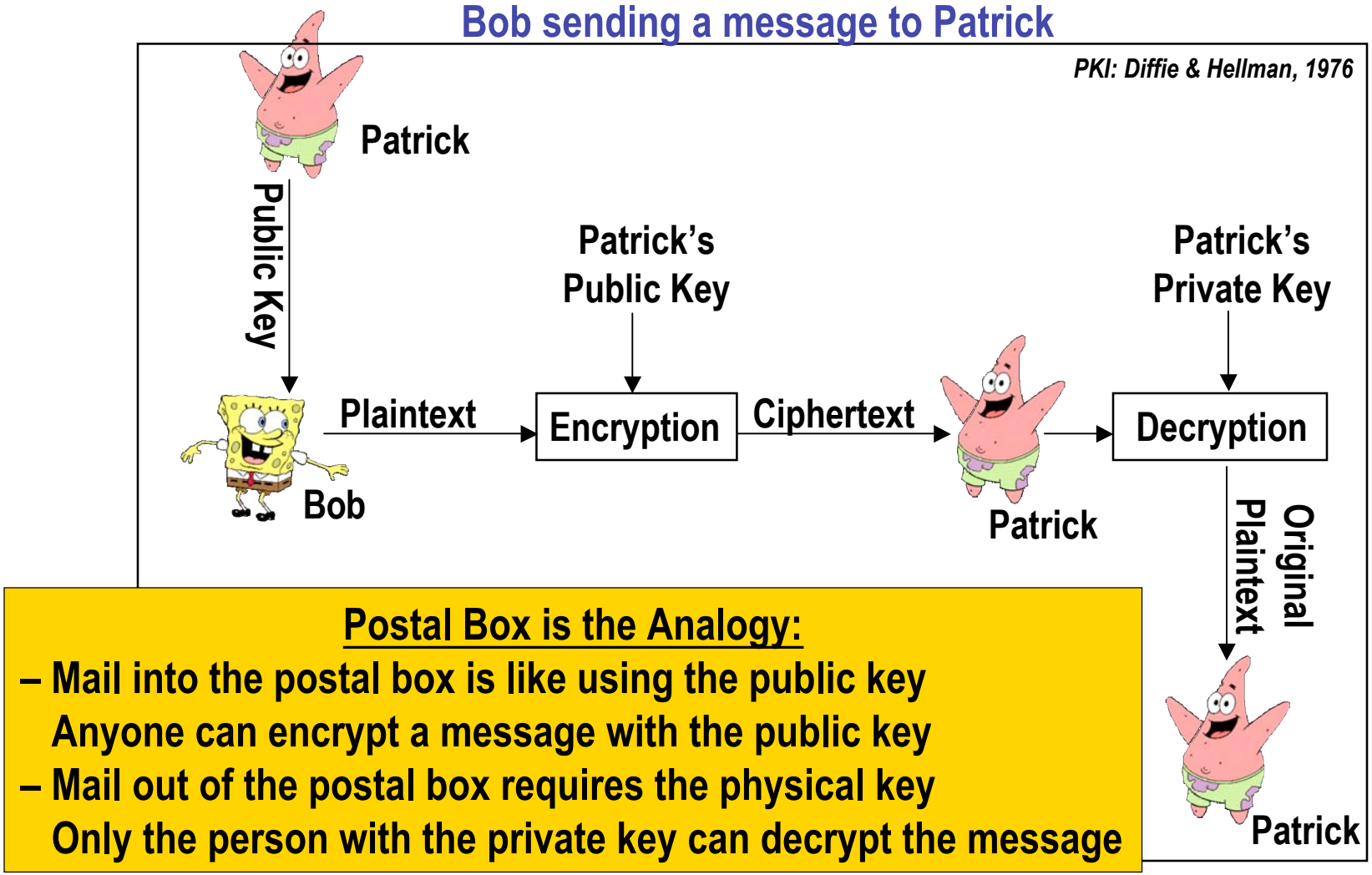


- Symmetric Algorithm or Shared-Key Communication
  - Sender and receiver must agree on a key before they can communicate securely
  - Analogy is placing the message in a safe with one combination (key)

Security rests in the key:
- Divulging the key means that anyone can encrypt or decrypt messages
- Key management problem

GENERAL ATOMICS

PUBLIC-KEY CRYPTOGRAPHY PRESENTS AN EASIER TO MANAGE SOLUTION THAT SCALES TO LARGE GROUPS



Postal Box is the Analogy:

- Mail into the postal box is like using the public key
  Anyone can encrypt a message with the public key
- Mail out of the postal box requires the physical key
  Only the person with the private key can decrypt the message

GENERAL ATOMICS

IN PUBLIC-KEY CRYPTOGRAPHY COMPUTATIONALLY HARD TO DEDUCE THE PRIVATE KEY FROM THE PUBLIC KEY

- Anyone with a public key can encrypt a message but not decrypt
  - Only the person with the private key can decrypt the message

- Mathematically based on trap-door one way function (e.g. prime factorization)
  - Encryption is the easy direction, instructions are the public key
  - Decryption is the hard direction, even with large computers, unless the trap-door or secret (private-key) is known (f[p,q]=pq)

Easy Direction
(Public Key)

Hard Direction
Easier with the instructions
(Private Key)

For more information: *Applied Cryptography: Schneier, 1996*

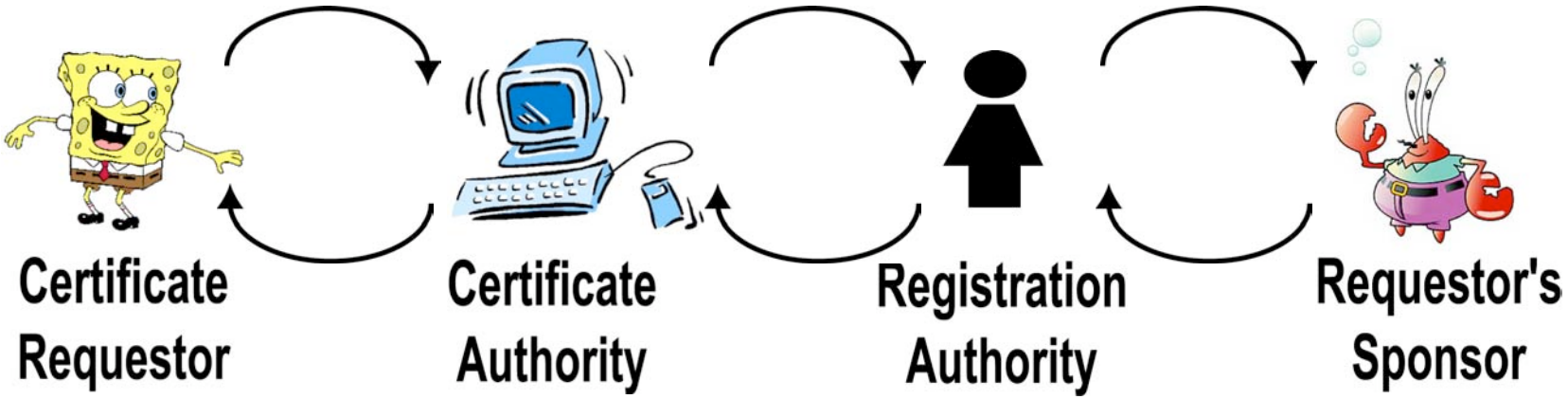
Secure Shell (SSH) uses public-key cryptography

GENERAL ATOMICS

PUBLIC-KEY INFRASTRUCTURE (PKI) IS A TECHNOLOGY TO DISTRIBUTE AND USE ASYMMETRICAL KEYS

- PKI gives trust that the public key being used truly belongs to the person (or machine) with whom/which they wish to communicate

- Certificates = Public Key + Trust
  - Binds a public key to identifying information about its owner
  - Managed for the benefit of all within the community of use

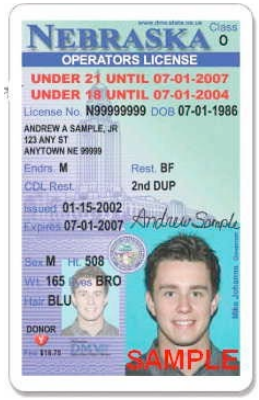


PKI foundation defined in ITU-T X.509 Recommendation

GENERAL ATOMICS

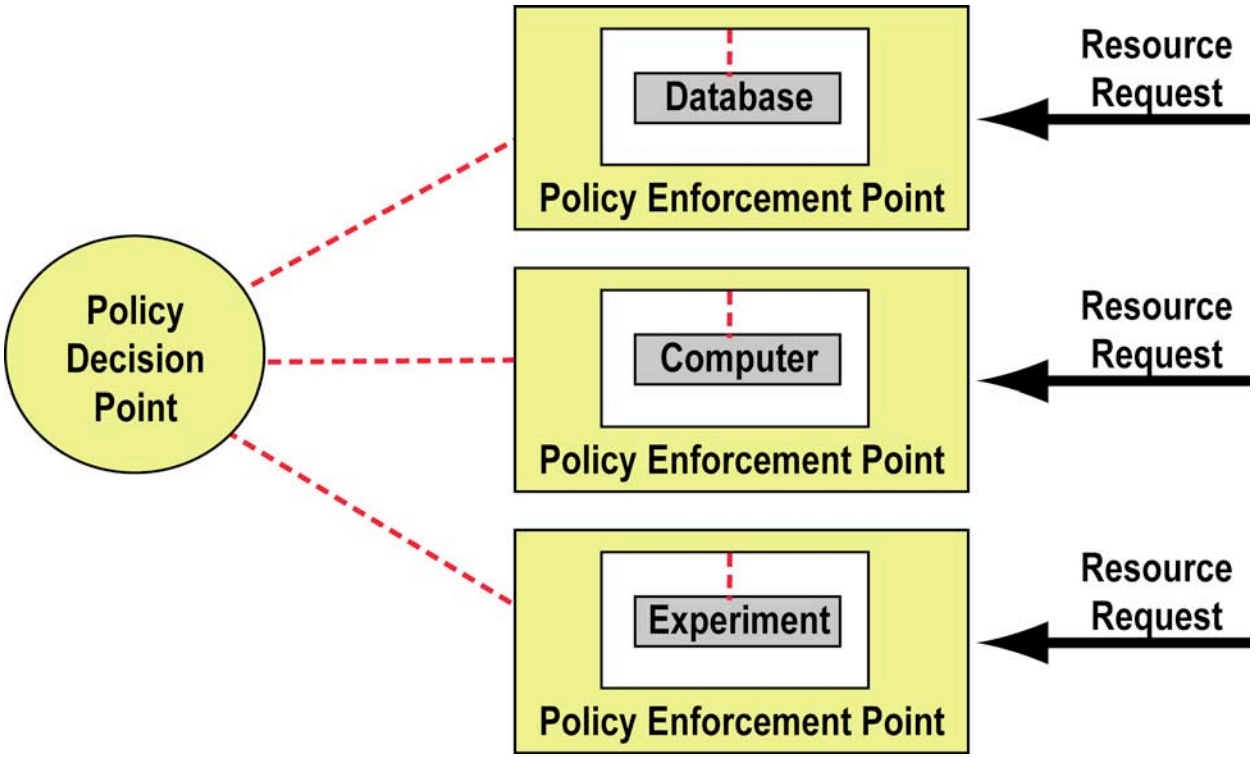
AUTHORIZATION: PROVIDE ASSURED, POLICY-BASED ACCESS CONTROL FOR COMPUTER MEDIATED RESOURCES

- After authentication, do they have rights to use the requested resource?
  - Authorization Policy
  - Must be solved in a Grid environment (multiple resource providers)
- Policy Decision Point (PDP)
  - A component deciding what access a user is allowed to a resource
- Policy Enforcement Point (PEP)
  - A component allowing/denying access to a resource (enforce decision)
- Attributes of User and Resources
  - Characteristics determine access (e.g. group membership, disk quota)



GENERAL ATOMICS

AUTHORIZATION: CENTRALIZED POLICY DECISION POINT FOR DEFINING RESOURCE USAGE



- It is the authorization policy that frames the Virtual Organization
  - Who can do what, where, and when

DATA MANAGEMENT

- Motivation for Collaborative Research
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GENERAL ATOMICS

DATA MANAGEMENT: THE RELATIONSHP BETWEEN REAL WORLD OBJECTS AND THEIR ASSOCIATIONS

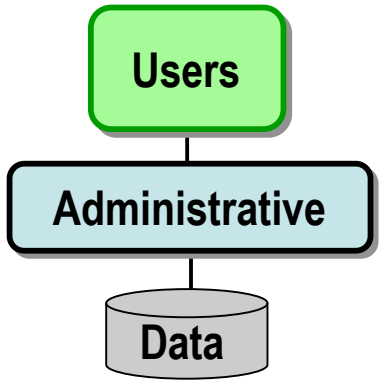
- Database
  - Collection of highly structured data
  - Along with a set of access and control mechanisms
- Provide users with a meaning-based view of data
  - Shield from irrelevant detail
- Support operations on data
  - Queries, updates (SQL: structured query language)
- Provide data control
  - Integrity, protection
  - Concurrency, recovery

Airline database a prime example

GENERAL ATOMICS

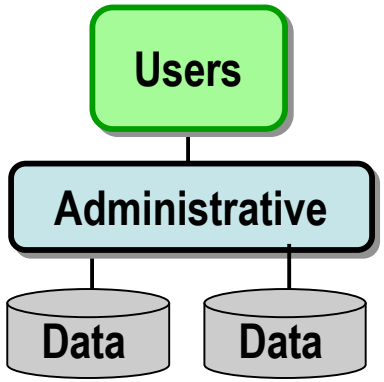
EVOLUTION OF DATA MANAGEMENT

- Collection - managed data
  - Use database to organize attributes about data objects
  - Separate information management from data storage
  - Support APIs for information discovery, data access



Integration from a data handling system which characterizes the storage systems

- Distributed data collection
  - Same name space and same data model
  - Separate administrative domains
  - Heterogeneous database instances

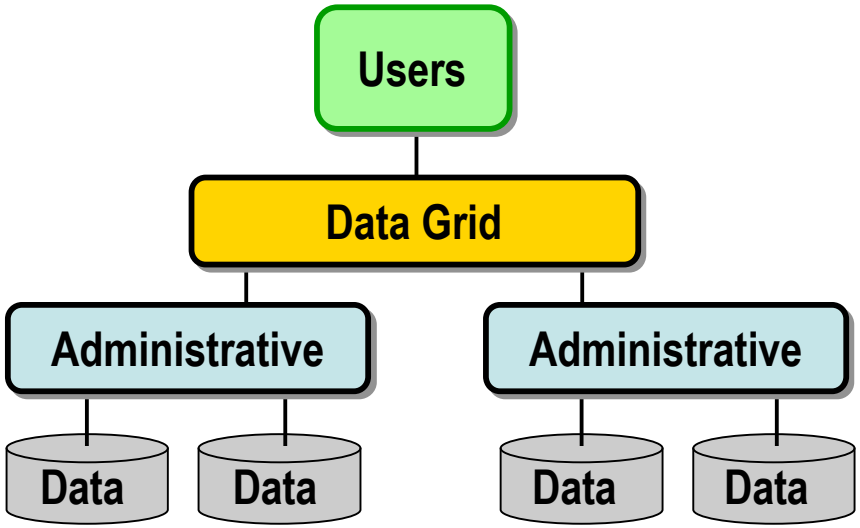


Integration requires the ability to characterize both the schemas and the table structures of each information repository

DATA MANAGEMENT IS FUNDAMENTAL TO GRIDS

- Data Grid - linking multiple data collections
  - Separate name space, physical location, administrative control, data model

- Data grid is a collection that provides mechanisms to hide latency and manage semantics



GENERAL ATOMICS

WALMART AS AN EXAMPLE OF THE BENEFITS OF EFFICIENT DATA MANAGEMENT

WAL★MART®
ALWAYS LOW PRICES. Always.

"The emergence of retailing giants such as Wal-Mart Stores Inc. stems directly from the deployment of sophisticated electronics to run a huge supply and distribution network."
– WSJ 8/29/95

- Point-of-sale distribution technology
- Sale in a store is also a real-time database transaction
- Both store inventory and supplier purchase request
- Testing to Radio Frequency Identification (RFID)
  - Security & inventory in real-time at the shelf

RFID Tag

GENERAL ATOMICS

SCIENTIFIC DATA IS MORE COMPLICATED

- Specialized data types and methods
  - Data model and query support
  - Physical organization & data structures
- Complex data model
  - Complexity of defining, viewing, and querying
  - Support over commercial software
  - Data model evolution
- Very large datasets
  - Many terabytes
  - Conventional index structures don't scale
  - Access from tape or parallel disks

GENERAL ATOMICS

DATA GRIDS FOR HIGH ENERGY PHYSICS: COMPACT MUON SOLENOID (CMS) AT THE LHC IN CERN

1800 Physicists, 150 Institutes, 32 Countries

~PBytes/sec

Online System

~100 MBytes/sec

Offline Processor Farm
~20 TIPS

1 TIPS is approximately 25,000 SpecInt95 equivalents

~100 MBytes/sec

CERN
Computer Center

~2.5 Gbits/s

Tier 0

Tier 1

Other National
Regional Centers

Italy
Regional Centers

FermiLab ~4 TIPS

~0.6 - 2.5 Gbps

Tier 2

Caltech
~1 TIPS

Other Tier2 Centers
~1 TIPS

~622 Mbits/sec

Tier 3

Other Institutes
~0.2 TIPS

Physics data cache

~100 - 1000 Mbits/s

Tier 4

Physicist workstations

There is a "bunch crossing" every 25 ns
There are 100 "triggers" per second
Each triggered event is ~1 MByte in size

GENERAL ATOMICS

COMPUTING AND VISUALIZATION

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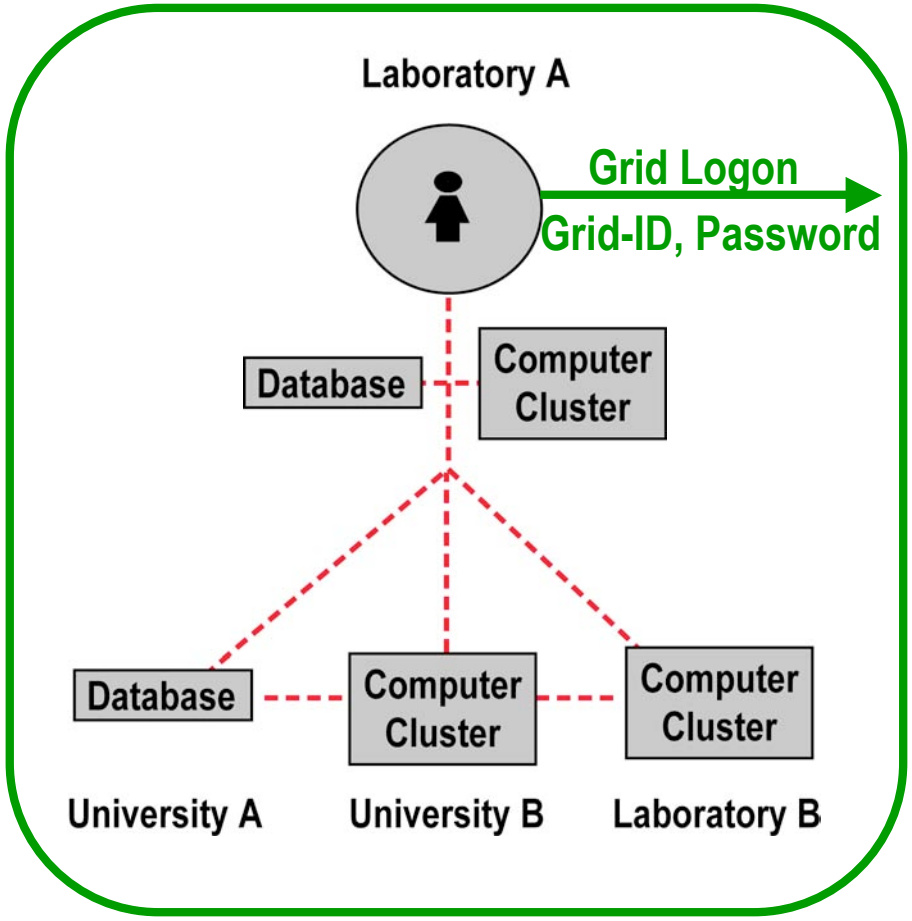
GENERAL ATOMICS

GRID COMPUTING FACILITATES USAGE OF COMPUTATIONAL RESOURCES WITHIN VIRTUAL ORGANIZATIONS



Virtual Organization A

- Single sign-on security model
  - Credential delegation
- Automatic resource discovery
- Resource and job monitoring
- Data Management

GENERAL ATOMICS

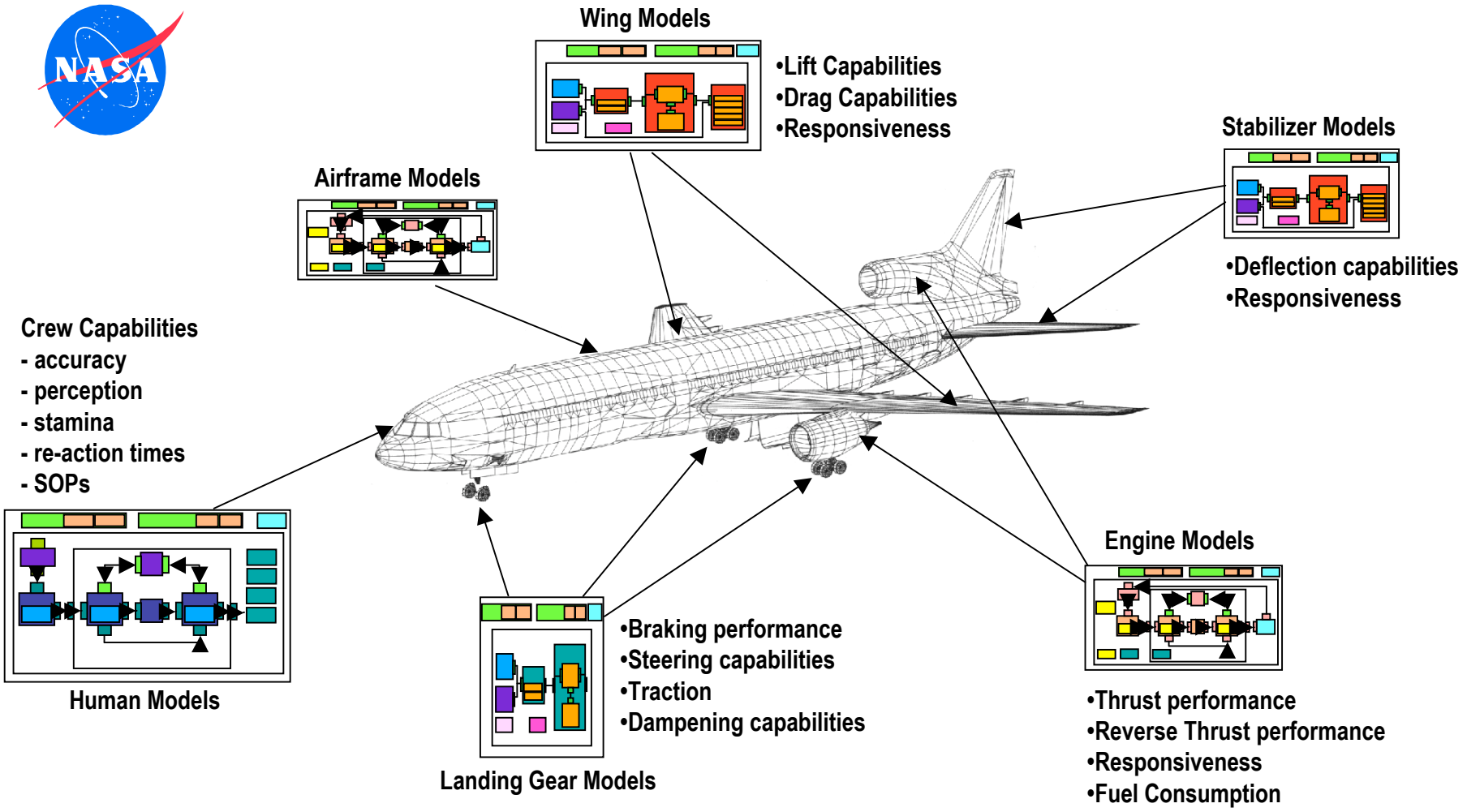
ROYAL DUTCH/SHELL: COMMERCIALLY DEPLOYED GRID COMPUTING

- Subsurface exploration
  - Up to $25K/sq-mi
- On-demand Grid computing
  - Seismic interpretation
- Improves accuracy of data analysis
  - Reduces processing time
- Employees focus on the key science

"Grid computing is important to Shell because it offers the potential to create truly unlimited resource, with a uniform interface to a variety of services."
J. Buur, Physicist, Shell International

GENERAL ATOMICS

NASA DISTRIBUTED GRID COMPUTING: INFORMATION POWER GRID FOR AVIATION SAFETY



Whole aircraft simulation in operational environments produced by coupling all of the sub-system simulations

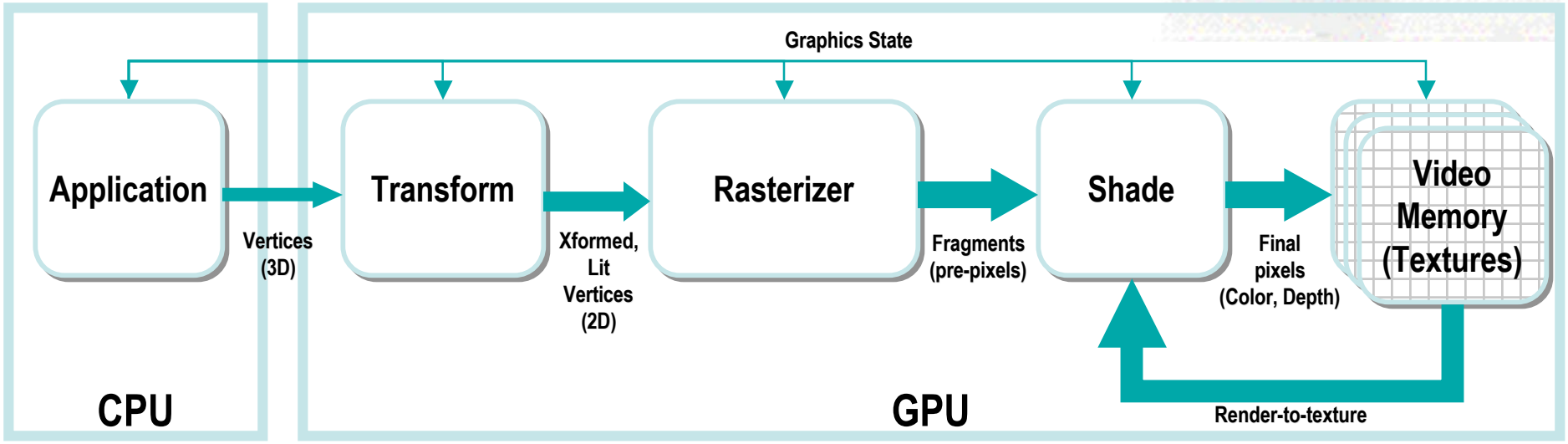
GENERAL ATOMICS

VISUALIZATION OF SCIENTIFIC DATA IS CRITICAL FOR UNDERSTANDING

- Graphical representation of data to gain understanding and insight

- Growing demands imply specialized hardware/software
  - Video game industry has been a big driver

The Graphics Pipeline



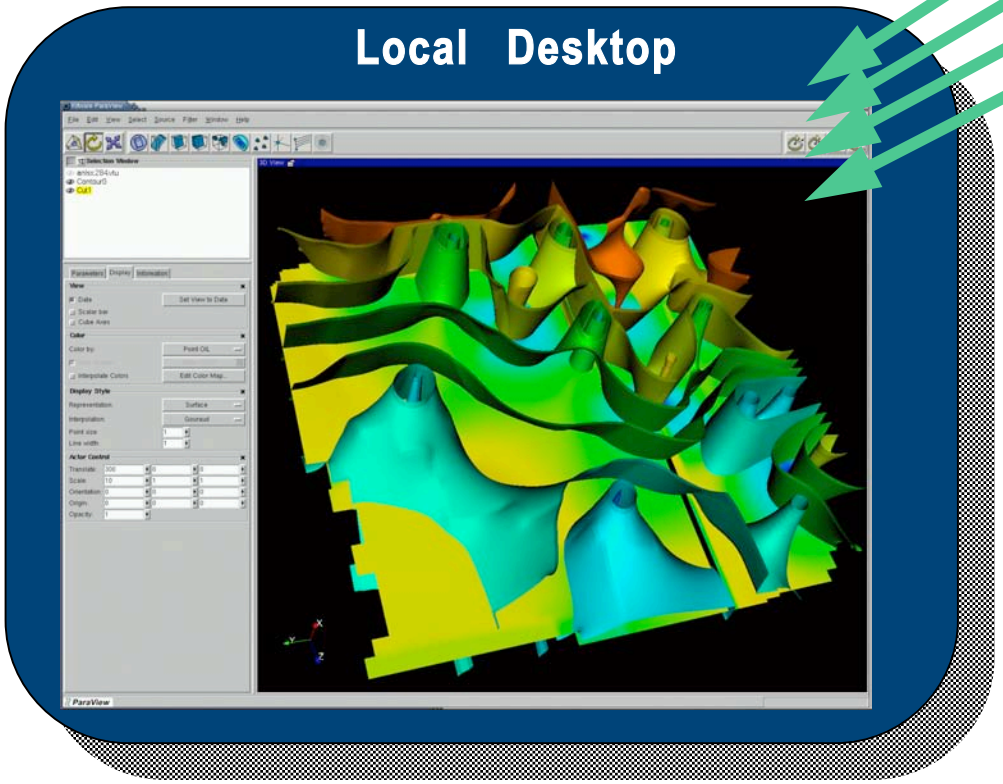
GENERAL ATOMICS

GRID BASED PARALLEL RENDERING FOR LARGE DATASETS

- Large amount of data
- Compute intensive rendering
- The need for interactivity

Render Farm

Local Desktop

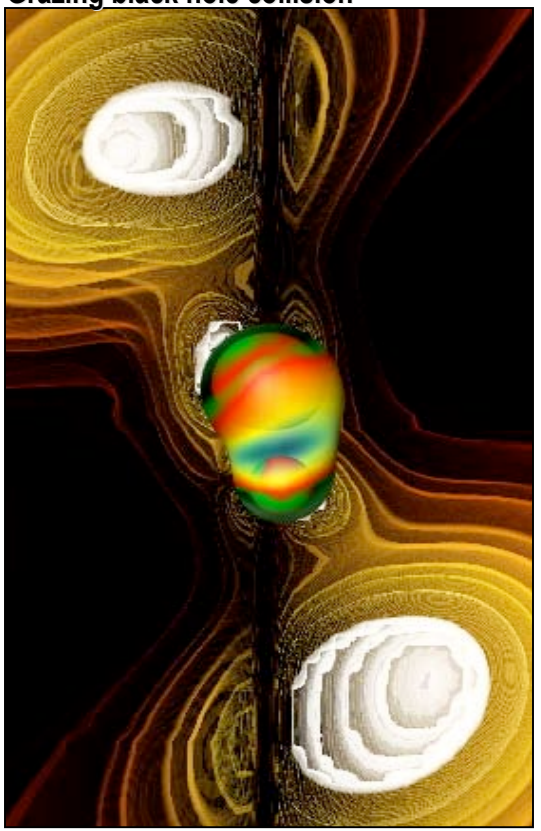


- ParaView from Kitware
- TeraGrid is deploying
- TB to MB for visualization
- Intelligent CPU/network usage
  - Process & render remotely
  - Process remote/render local

GENERAL ATOMICS

ENABLING GRID VISUALIZATION SERVICES IS CHALLENGING

Grazing black hole collision



- Numerous approaches
  - Do everything on the remote server
  - All but the rendering on the remote server
  - Use a local proxy for rendering
  - Do everything locally
- Grid visualization resources are limited
  - An easy way to grid-enable existing packages
- Grid resources heterogeneous wrt visualization
  - Programs need to be performance-portable and dynamically configurable
- Grid resources can be dynamic
  - Might need user interaction (e.g. accuracy versus frame rate)

GENERAL ATOMICS

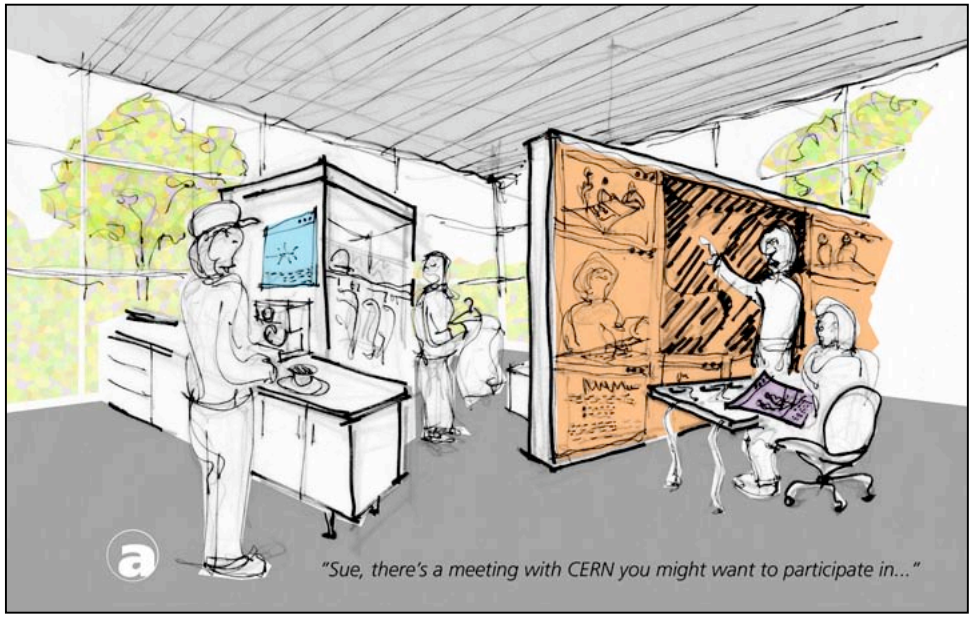
ADVANCED COLLABORATIVE ENVIRONMENTS (ACE)

- Motivation for Collaborative Research
  - Science is more and more a team activity
- Grid Computing
  - Resource sharing and coordinated problem solving in a virtual organization
- Security
  - Allowing stakeholders to control resources they give to the Grid
- Data Management
  - Where is that piece of data?
- Computing and Visualization
  - Graphical representation of data to gain understanding and insight
- **Advanced Collaborative Environments (ACE)**
  - **Productive distributed group work**
- Grid and ACE technologies applied to fusion research
  - The National Fusion Collaboratory Project

GENERAL ATOMICS

ADVANCED COLLABORATIVE ENVIRONMENTS: AD HOC COLLABORATION AND DISTRIBUTED INVESTIGATION

- **Goals**
  - Create group work productivity benefits comparable to that of radical (classical) collocation for distributed work
- **Persistence**
  - Can Persistent Shared Spaces enable cost-effective support of Virtual organizations?
- **Presence**
  - The "sensation of being there"
- **Immersion**
  - Coupling communications channels to sensory modalities



High-degree of Immersion ⇒ increased presence
High-degree Presence ⇒ increased sense of collocation

GENERAL ATOMICS

COMMERCIAL "COLLABORATIVE ENVIRONMENTS"

Simple camera at the low cost end

GENERAL ATOMICS

COMMERCIAL "COLLABORATIVE ENVIRONMENTS"

Video Conferencing Systems at the high cost end

GENERAL ATOMICS

RESEARCH ON INTERNET BASED MULTI-USER ADVANCED COLLABORATIVE ENVIRONMENTS

- **Access Grid**
  - Enabling group-to-group Collab
  - Complex application sharing
  - Affordable IP based audio/video
  - Scalable: laptop to large room
  - 300+ Room-based systems
  - Example: SER-CAT on APS

- **VRVS**
  - Web oriented
  - Video Conf and Collaboration
  - Over IP based networks
  - 106 countries
  - Example: High Energy Physics

GENERAL ATOMICS

CHEVRON–TEXACO DEPLOYING ACCESS GRID NODES TO SUPPORT WORLDWIDE OIL EXPLORATION

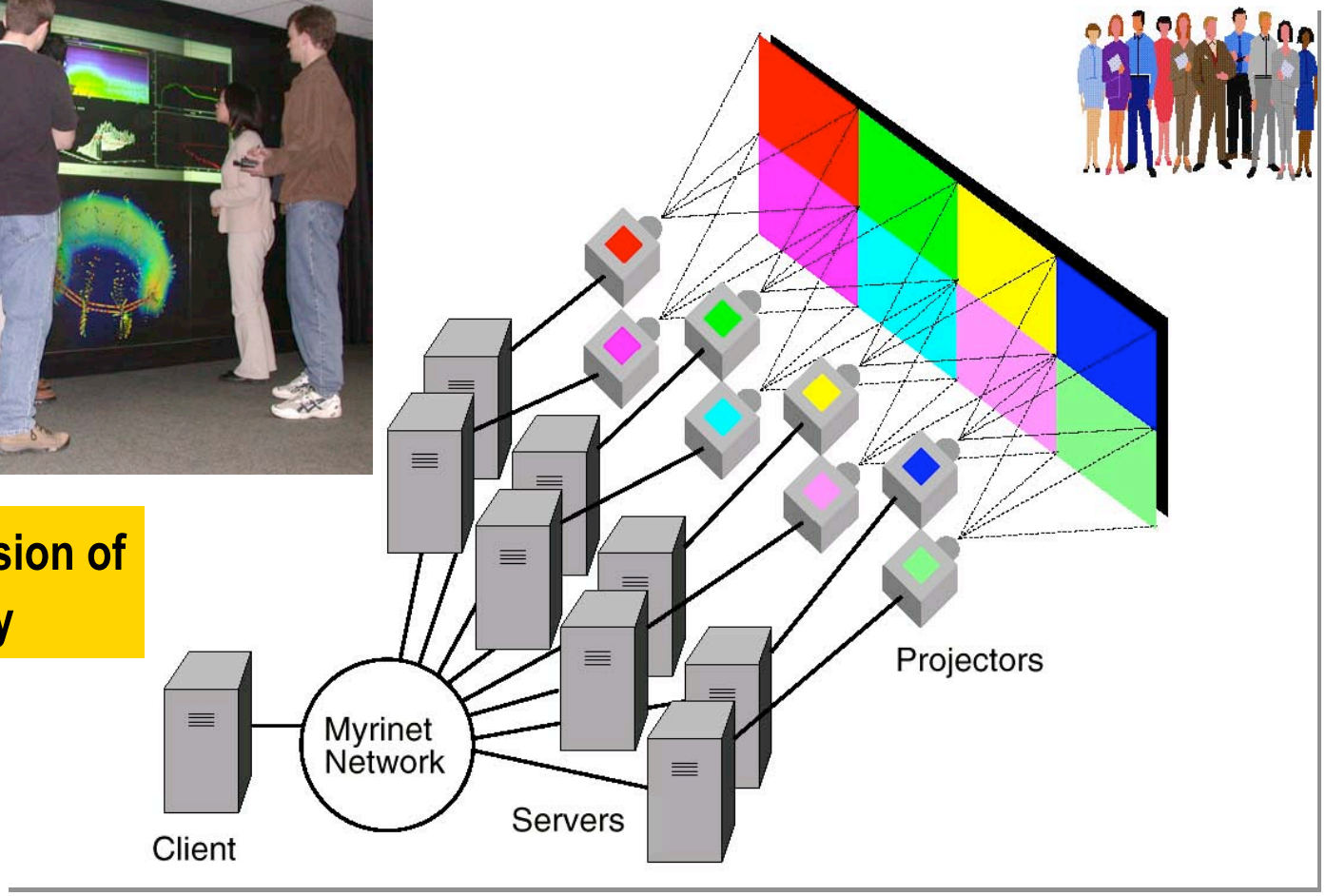
- Oil rigs & drilling ships in the field
- Analysis & decision room back home
- 18+ nodes over wired & satellite
- Expanding to Africa land drilling
- inSORS doing actual deployment work

inSORS®

GENERAL ATOMICS

TILED DISPLAY WALLS: LARGE FORMAT ENVIRONMENT FOR HIGH RESOLUTION AND LARGE GROUP VISUALIZATIONS

Creating the illusion of one display



GENERAL ATOMICS

THE NATIONAL FUSION COLLABORATORY PROJECT

- Motivation for Collaborative Research
  - Science is more and more a team activity
- Grid Computing
  - Resource sharing and coordinated problem solving in a virtual organization
- Security
  - Allowing stakeholders to control resources they give to the Grid
- Data Management
  - Where is that piece of data?
- Scientific Computing and Visualization
  - Compute and see the data for understanding
- Advanced Collaborative Environments (ACE)
  - Productive distributed group work
- Grid and ACE technologies applied to fusion research
  - The National Fusion Collaboratory Project

GENERAL ATOMICS

THE NATIONAL FUSION COLLABORATORY PROJECT

- Funded by the DOE Office of Advanced Scientific Computing Research
  - Part of the SciDAC initiative
- Unify distributed MFE research into a U.S. Virtual Organization

GOALS

- More efficient use of experimental facilities
- Integrate theory and experiment
- Facilitate multi-institution collaboration
- Create standard tool set

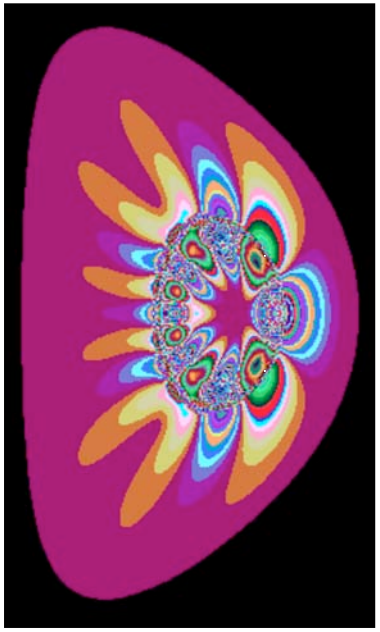
Office of Science
U.S. DEPARTMENT OF ENERGY

ASCR

SciDAC
Scientific Discovery through Advanced Computing

GENERAL ATOMICS

THE VISION FOR THE NFC'S TECHNOLOGIES



- Data, Codes, Analysis Routines, Visualization Tools should be thought of as network accessible services
  - Access is stressed rather than portability
  - Transparency and ease of use are crucial elements
  - Not CPU cycle scavenging or "distributed" supercomputing

- Shared security infrastructure with distributed authorization and resource management
  - Ease of use: "security with transparency"
  - X.509 certificates from a trusted Certificate Authority
  - Distributed authorization allows stakeholders to control their resources

- Collaborative nature of research requires shared visualization applications and widely deployed collaboration technologies
  - Integrate geographically diverse groups

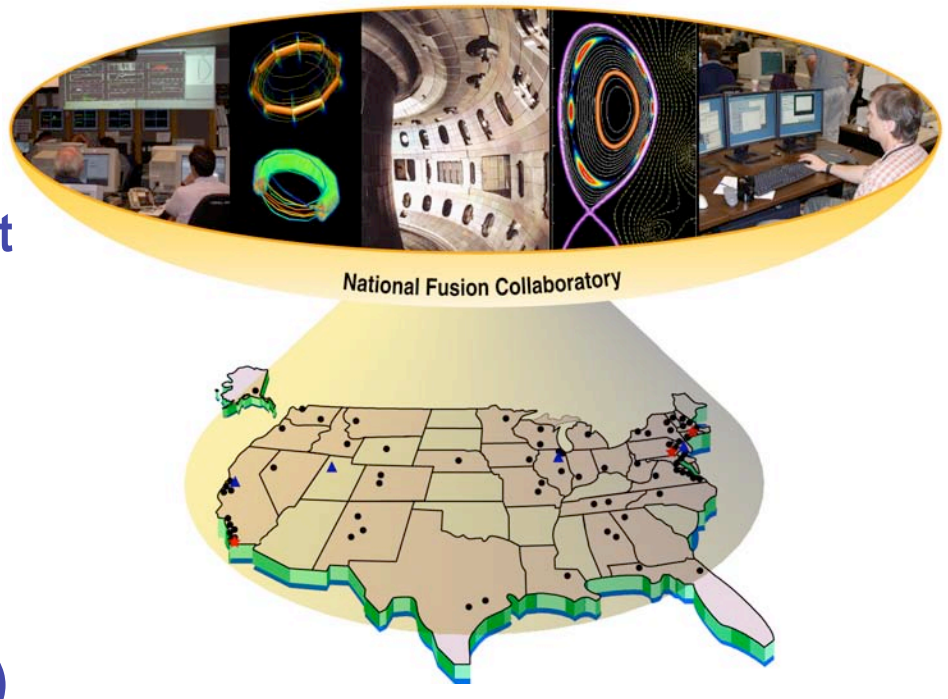
Optimize the most expensive resource - people's time

FusionGRID www.fusiongrid.org

GENERAL ATOMICS

FUSIONGRID: SECURE ACCESS TO RESOURCES

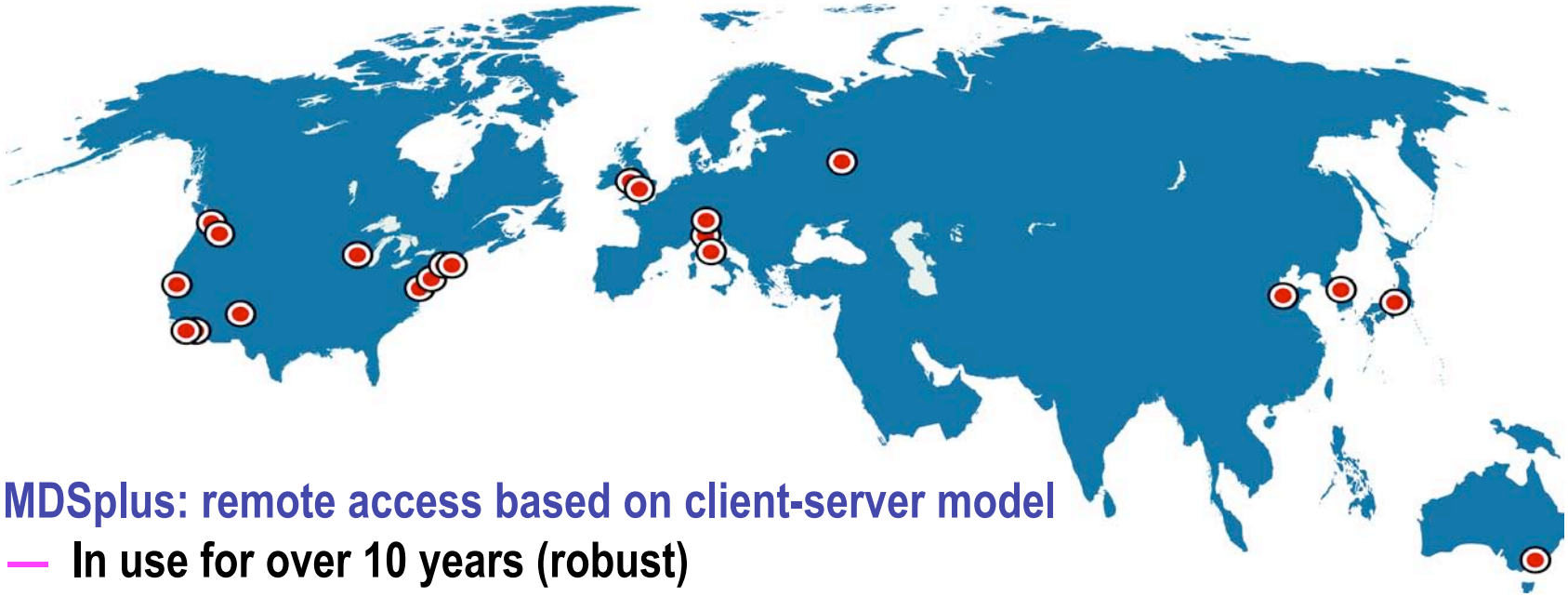
- Authentication: PKI via X.509 certificates
  - FusionGrid CA
  - FusionGrid RAs (Humans)
- Centralized certificate management
  - MyProxy server
  - More secure & easier for user
- Onetime FusionGrid login
  - Globus toolkit
- Authorization: Customized (ROAM)
  - All resources call central Policy Decision Point (PDP)
  - Policy for all resources in a relational database



FusionGRID
www.fusiongrid.org

GENERAL ATOMICS

FUSIONGRID: SECURE ACCESS TO FUSION DATA



- MDSplus: remote access based on client-server model
  - In use for over 10 years (robust)
- Wide adoption worldwide
  - Unified data interface (e.g. Visualization)

Not yet a unified U.S. fusion data Grid

- MDSplus data access now can be secure
  - FusionGrid authentication (Globus GSI with X.509 certificates)
  - FusionGrid authorization (ROAM)

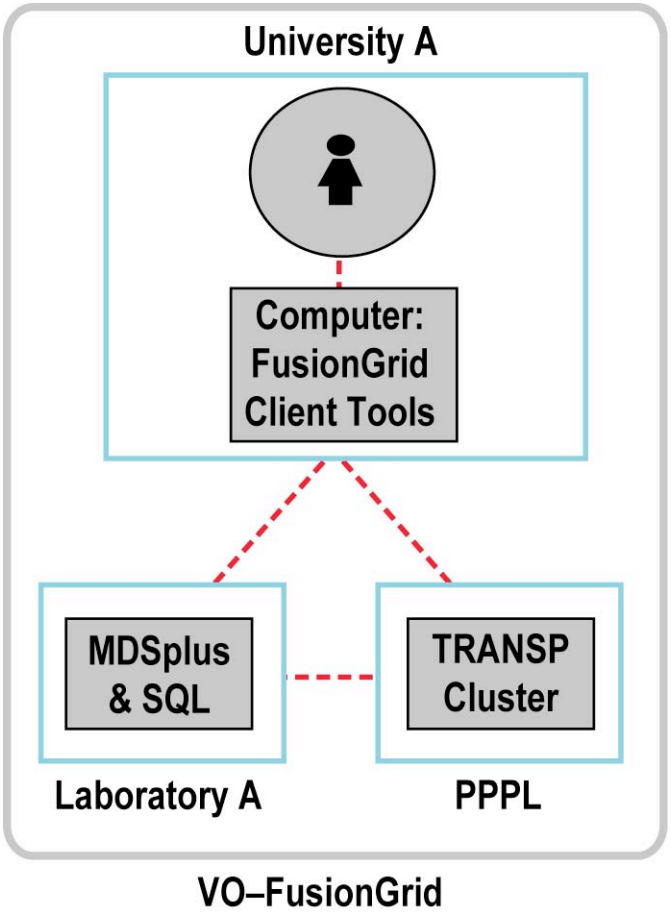
FusionGRID www.fusiongrid.org

GENERAL ATOMICS

TRANSP: SUCCESSFUL GRID COMPUTING FOR FUSION SCIENCE

One physical installation of TRANSP

- The U.S. TRANSP Service
  - 4,700 cases, 20,000 CPU hours
  - 10 fusion experimental machines
- Centralized expertise for better support
  - Debugging, maintenance,monitoring
- Reduced administration work at other labs
  - Smaller sites to use bigger codes
- Model for other codes
  - MHD code GATO released



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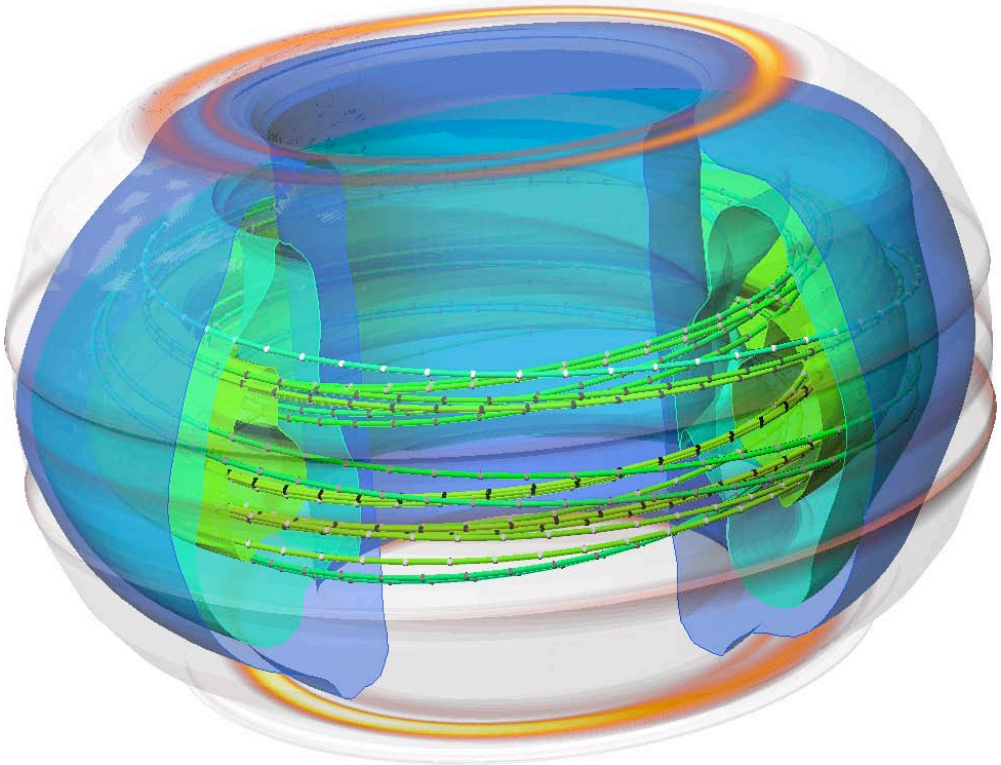
GENERAL ATOMICS

SCIRUN TO VISUALIZE COMPLEX SIMULATIONS FOR BETTER UNDERSTANDING

- Open source, multi-platform capable for a wide user base
- To facilitate quantitative comparison of simulations and experimental results



SciDAC CEMM NIMROD Simulation of a DIII–D Plasma

Raising the challenge of very large datasets
- **MDSplus**
- **Storage method**
- **Data location**
- **Parallel I/O**

Not Grid-based rendering

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GENERAL ATOMICS

TILED DISPLAYS INSTALLED IN FUSION CONTROL ROOMS

DIII–D Tokamak Control Room

NSTX Tokamak Control Room

- Enhanced collaboration within a large control room
  - "Publish" your analysis for the group to see and discuss
- Share and collaborate between tiled displays
  - Clone of tokamak control room (discussed for ITER)

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GENERAL ATOMICS

ACCESS GRID: REAL TIME COMPLEX COMMUNICATION

Scientific Leadership of JET in UK from US

January 2004, San Diego

Remote Participation from JET to DIII–D

May 2004, DIII–D Tokamak Control Room

- Being used for seminars, working meetings, tokamak operations
  - Linux, Windows, and Macintosh OS X
- For tokamak operations, the collaborative control room
  - Human collaboration, shared data, shared applications, shared info

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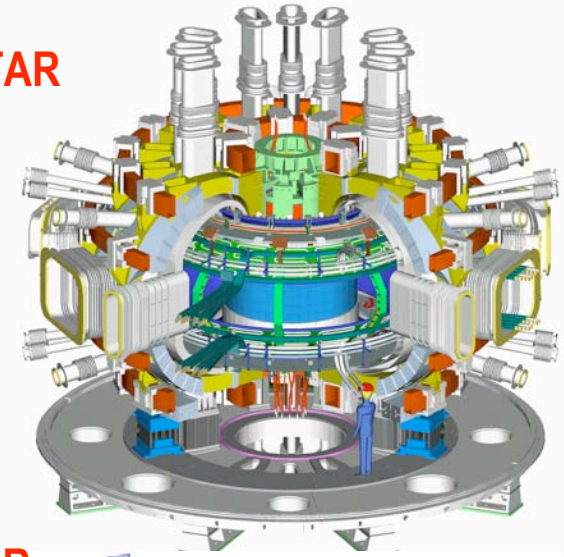
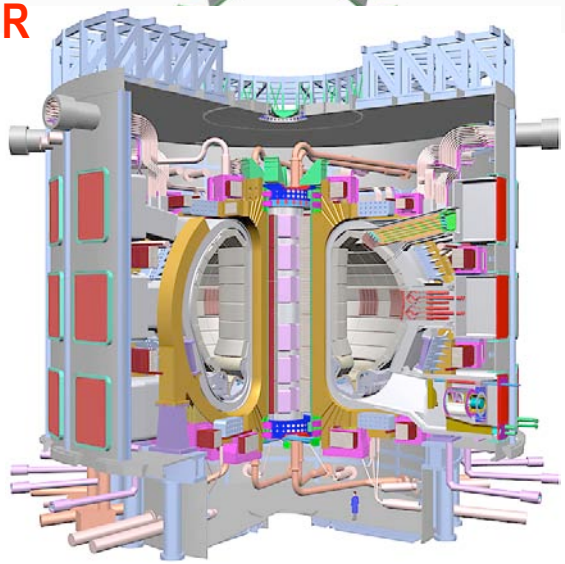
GENERAL ATOMICS

NFC TECHNOLOGIES SCALE TO THE NEXT DEVICE

KSTAR



ITER



- One physical location
  - International collaboration
- Pulsed experiment with simulations
  - ~TBs of data in 30 minutes
- Successful operation requires
  - Large simulations, shared visualization, decisions back to the control room
  - Remote Collaboration via FusionGrid
- Grid and ACE technologies critical to the success of these programs
  - Design, engineering, construction, & operations

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www.fusiongrid.org

GENERAL ATOMICS

AN EARLY OR CURRENT USER OF FUSIONGRID?

- We have learned a lot
  - Tackling ease-of-use
  - Numerous enhancements
- Stop by our display (Poster Room)
  - Talk to the experts
  - Learn & provide feedback
- To do at the display
  - Join FusionGrid (certificate)
  - Run a code on FusionGrid
  - Use an AG node
  - Interact with tokamak control room

FusionGRID
www.fusiongrid.org

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CONCLUSIONS AND PROSPECTS

- Large body of work being done on Grid computing and ACE
  - The fusion scientific domain should continue to take advantage
- Technology has broad applicability beyond tokamak plasma physics
  - Design, engineering, and construction of diagnostics and machines
  - Applicable to KSTAR and ITER during construction phase
- What will the virtual ITER laboratory in the U.S. be like?
  - Include construction activities, meetings, and the control room
  - Absolutely essential for the successful U.S. participation in ITER

First on our list is fusion. The prospect of limitless source of clean energy for the world leads with our commitment to join the international fusion energy experiment known as ITER.

– Secretary of Energy Spencer Abraham, November 10, 2003

Introducing the Department's 20-year plan for building the scientific facilities of the future.

GENERAL ATOMICS

STOP BY THE POSTER ROOM AND TRY THIS TECHNOLOGY YOURSELF!

POSTER ROOM:
Exhibit Hall A

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